Charging properties of the silicon / zinc oxide nanoparticle heterostructure

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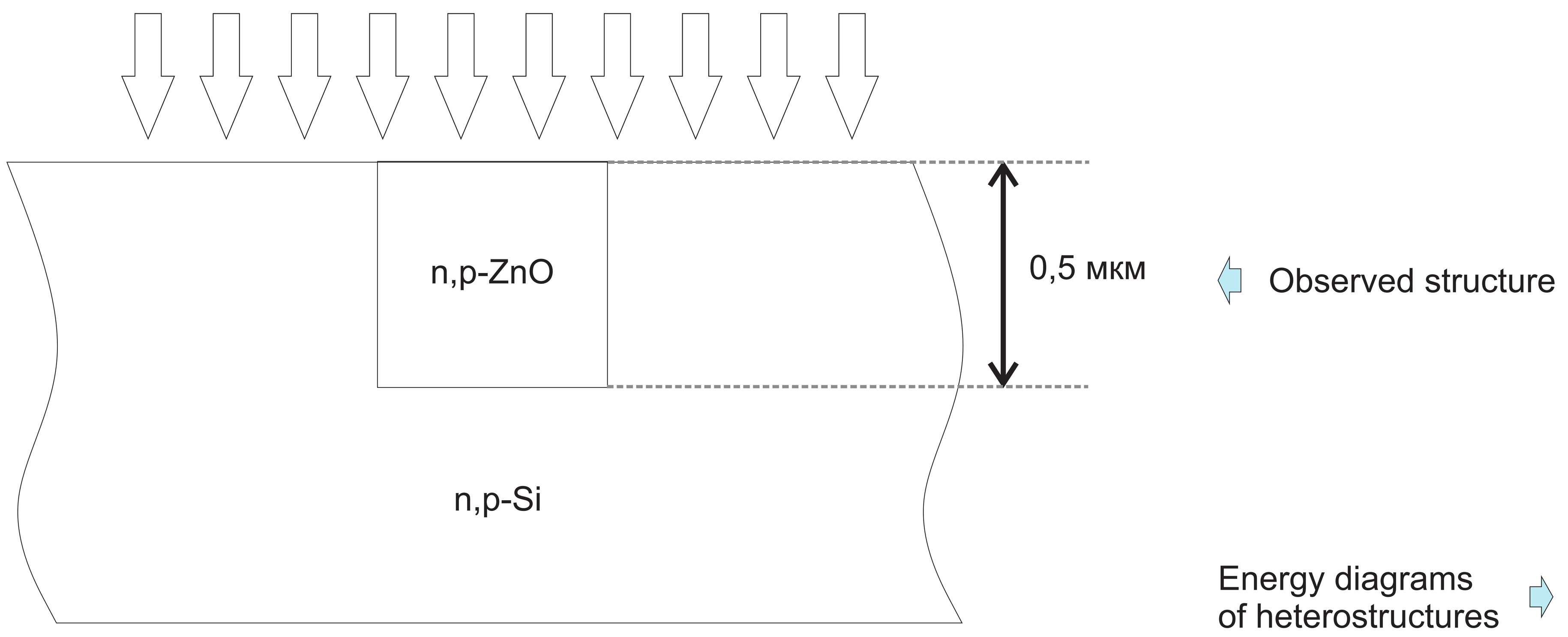
INTRODUCTION

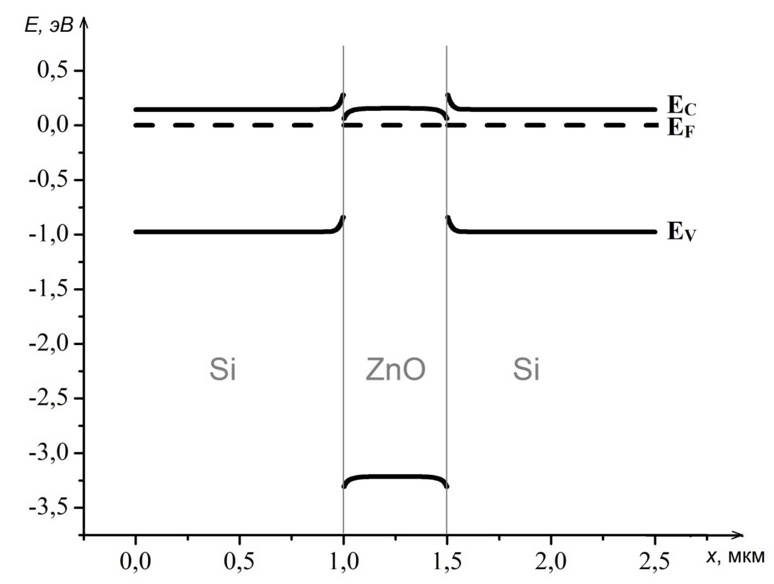
Zinc oxide ZnO is a semiconductor with a direct band gap of 3.37 eV at room temperature, which makes ZnO a promising material for use in many areas, such as photocatalytic water and air purification, photocatalytic water splitting, optoelectronics, gas sensors, gas sensors [1]. Zinc oxide also has a number of advantages over other materials used in photocatalysis: low cost, non-toxicity, low reflectance in the solar spectrum, the ability to create low-dimensional structures using chemical etching (amphotericity), resistance to high-energy radiation, flexible changing of electrophysical and optical properties by doping it with various impurities and controlling the conditions for its production [2]. The implementation of p-type ZnO is difficult because pure ZnO with a wurtzite structure naturally occurs in the form of an n-type semiconductor. It is caused by oxygen vacancies, excess zinc, and the presence of hydrogen atoms, [3].

MODEL

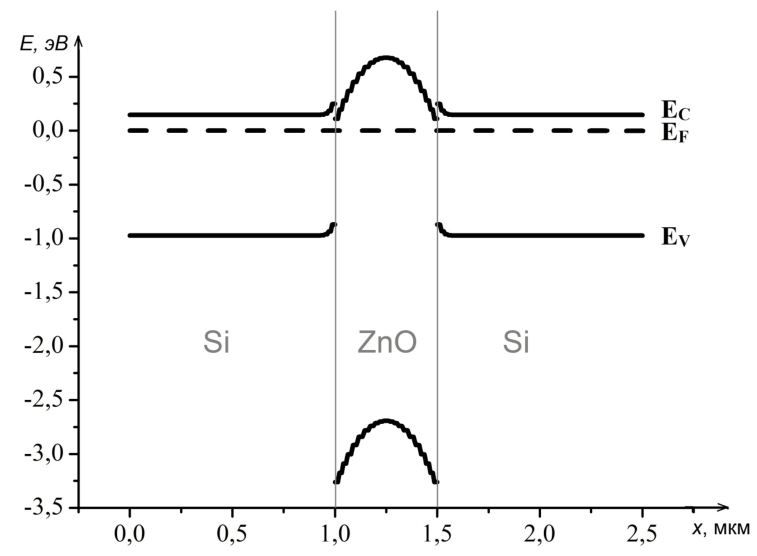
The Si/nanosized ZnO heterostructure was simulated using the Comsol Multiphysics software package. A two-dimensional diffusion-drift model of the heterostructure with the solution of the Maxwell system of equations was used. Properties of silicon [4] and zinc oxide [5] are shown in the table. The real and imaginary parts of the refractive index for silicon and zinc oxide were set in a table [6, 7].

		n,p-Si	n,p-ZnO
Eg, эВ		1,124	3,2
χ, эВ		4,05	4,8
ε		11,7	40
DOS, cm^{-3}	E_c	$2.8\cdot10^{19}$	$4.124\cdot10^{18}$
	E_v	$1.04\cdot10^{19}$	$1.138\cdot10^{19}$
$\tau_{n,p}$, мкс		10	$9,7\cdot10^{-4}$
μ_n, $см^2/(В\cdot с)$		1450	200
μ_p, $см^2/(В\cdot с)$		500	50
N_d, cm^{-3}		10^{17}	10^{16}

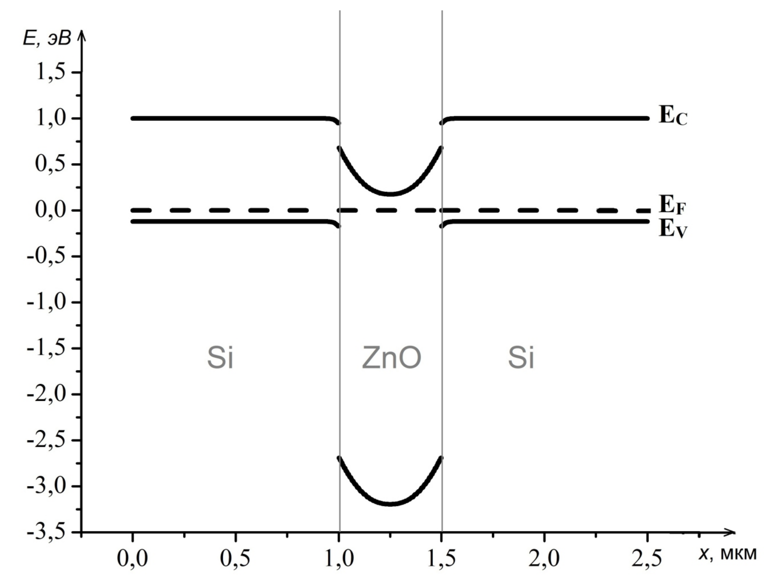




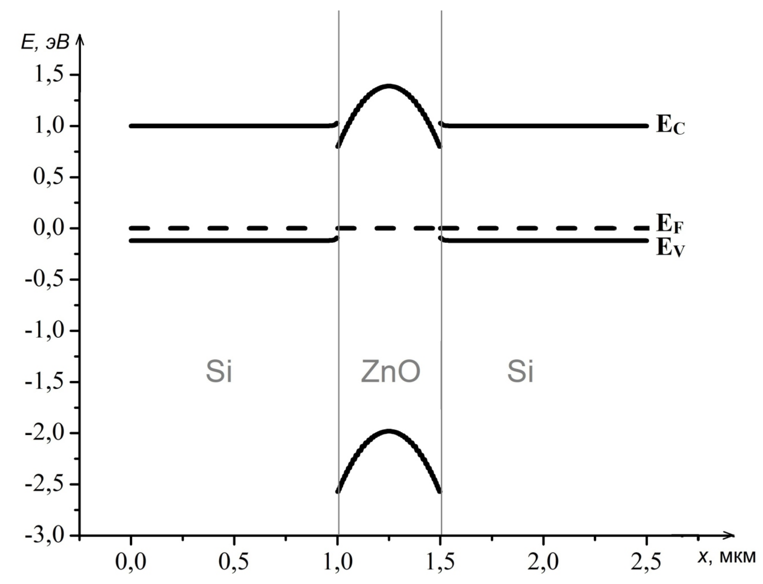
a - n-Si/n-ZnO



b - n-Si/p-ZnO



c - p-Si/n-ZnO

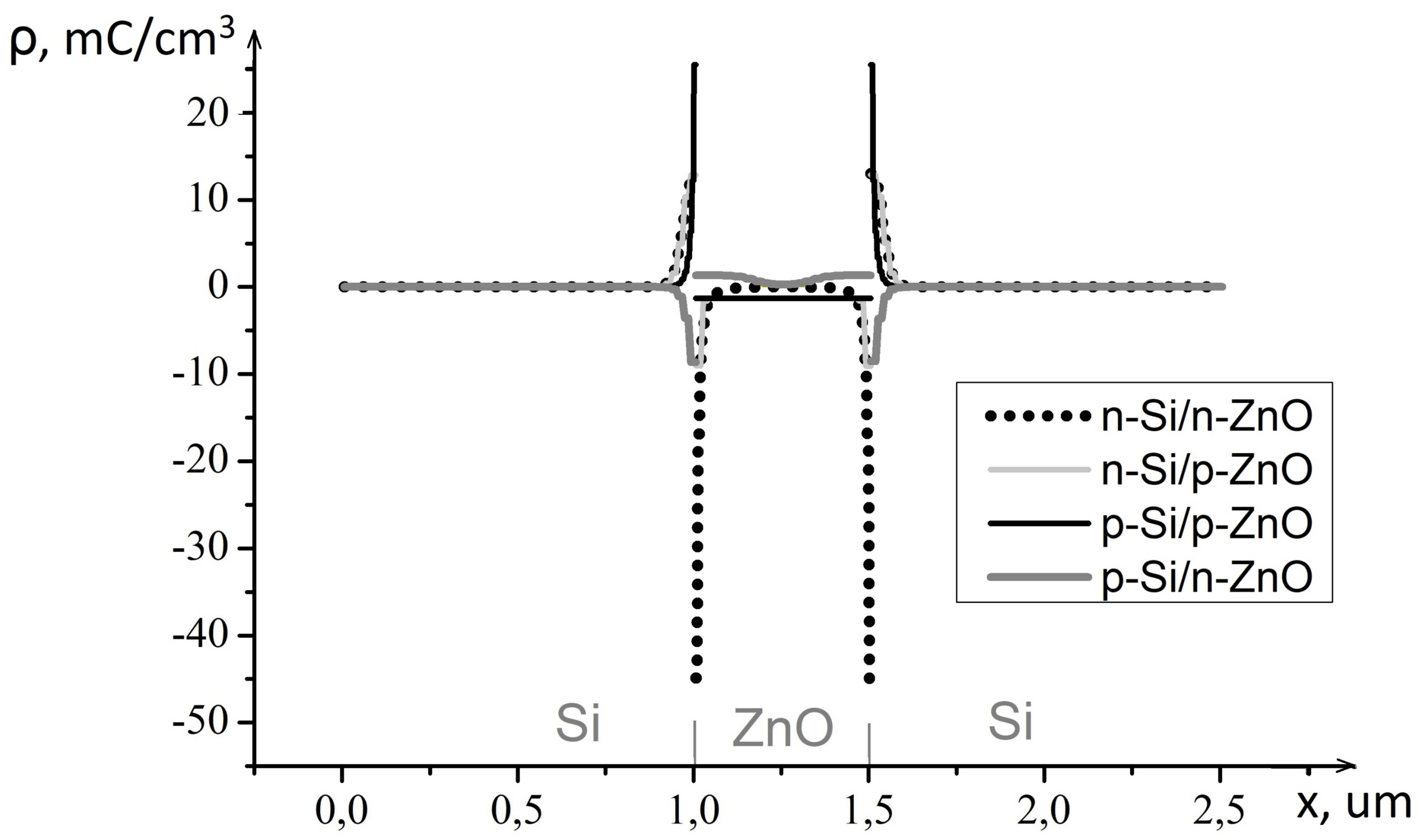


d - p-Si/p-ZnO

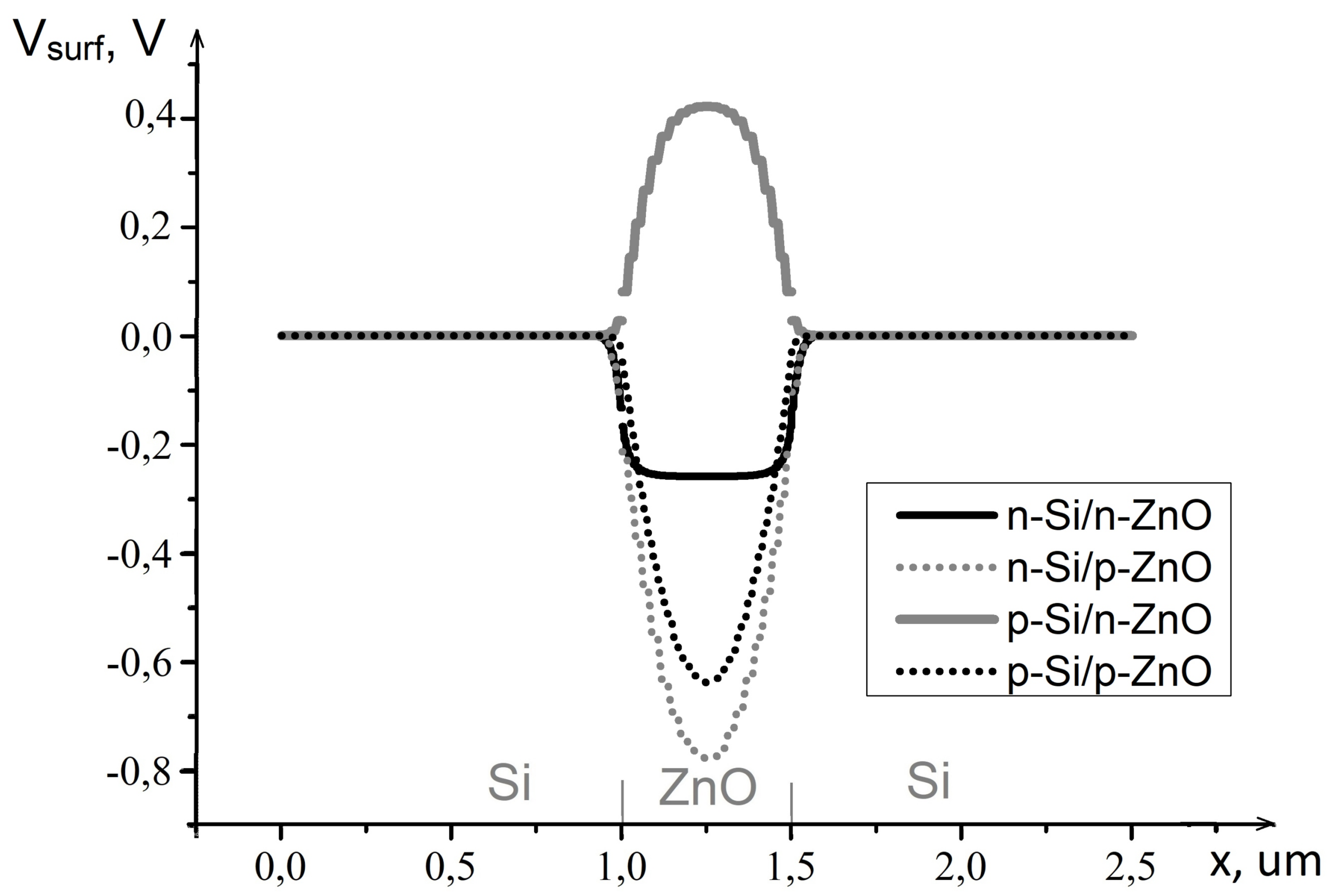
RESULTS AND DISCUSSION

The height of the barrier for electrons from the silicon side in the n-Si/n-ZnO heterostructure is 0.133 eV, after passing which they enter the region in zinc oxide enriched with electrons, thereby creating an excess negative charge at the the oxide nanoparticle zinc boundary (width ≈70 nm). The barrier for holes in the zinc oxide is 0.092 eV. In the n-Si/p-ZnO heterostructure, the barrier for electrons in silicon is 0.104 eV, and for holes in zinc oxide it is 0.567 eV. For the p-Si/p-ZnO heterostructure, these values are 0.028 eV and 0.57 eV, respectively. There are no such barriers in the p-Si/n-ZnO heterostructure which allows electrons generated in silicon and holes generated in zinc oxide to flow freely into another semiconductor.

Generation of charge carriers in ZnO occurs at wavelength <375 nm, in silicon at all wavelengths and it has a peak at ~950 nm. The generation is also observed in silicon under a ZnO particle at a



Electric charge density on the surface of heterostructures



Electric potential on the surface of heterostructures

CONCLUSIONS

Simulation of the charge properties and currents in zinc oxide nanoparticle in silicon heterostructures for cases of n- and p-types of conductivity demonstrated differences in the electric charge and potential on the surface of heterostructures without significant differences depending on the wavelength of incident radiation.

It is shown that the silicon / p-type zinc oxide nanoparticle heterostructure provides a negative potential and a negative surface charge on the surface of a zinc oxide nanoparticle regardless of the wavelength of solar radiation.

It opens up additional possibilities for the photocatalytic use of zinc oxide in a wider emission spectrum than its own absorption spectrum.

Achieving stable p-type conductivity of zinc oxide opens up many possibilities for creating optoelectric devices based on materials with a large conduction band. This will require better control over the natural n-type conductivity of zinc oxide which can compensate acceptor impurities.

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